

Analytical Data Treatment – Statistical and Numerical Analysis
CHEM 6120
The Ohio State University
Autumn 2022

Class Meeting: Monday/Wednesday/Friday 1:50-2:45
Location: 318 Bolz Hall

Instructor: Zachary Schultz
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Office Hours: Monday: noon-1:00 pm
Wednesday noon-1:00 pm
AND by appointment

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Office Hours: Monday: 3:00 pm – 4:00 pm, 311 Bolz Hall
Wednesday: 3:00 pm – 4:00 pm, 311 Bolz Hall

Course Description:

The course covers topics related to analyzing and comparing data obtained in scientific experiments. The topics covered in the course include: statistics, distributions, confidence intervals, hypothesis testing, analysis of variance, linear regression, smoothing, calibration, and multivariate analysis. This course will prepare you to determine if a result is significant.

Learning Goals:

- To develop a conceptual basis for understanding the principles of data processing, error analysis, and uncertainty as it relates to experimental chemical measurements.
- To develop a solid mathematical framework for implementing these principles of data processing and statistical analysis in the research setting.
- To convey the important role of statistical data analysis as it relates to ethical standards in research.

Text: There is no specific text assigned for this course. The material covered in this course is comprised from a number of sources. Some course readings will be posted to Carmen and announced in class. One goal of graduate school is to learn to find information independently. This course will build from both the primary literature and basic concepts. It will not follow a specific text; however, if you need a text: *Data Analysis for Chemistry – An Introductory Guide for Students and Laboratory Scientists* by Hibbert and Gooding, is recommended (a pdf version is available). Additionally, chapters from *Quantitative Chemical Analysis* by Harris will have background information relevant to topics covered in this course.

CARMEN will be used to post lecture notes, grades, as well as additional course materials of interest. Course announcements will be distributed using the roster in Carmen as well. Zoom links for lectures and Dr. Schultz's office hours are available on Carmen. We will attempt to simulcast lectures on zoom and in person. The zoom session will be recorded and made available on Carmen, if possible.

Tentative Course Schedule:

Dates	Topic
Aug. 24 – Aug. 29	Statistical Description of Data
Aug. 31- Sep. 5	Hypothesis Testing & Equivalence
Sep. 7 - Sep. 14	Least Square Regression - Calibration
	Exam 1 will be held Sept. 16
Sep. 19 - Sep. 23	ANOVA
Sep. 26 – Sep. 30	Design of Experiment
Oct. 3 – Oct. 10	Multivariate Analysis
Oct. 12	Final Exam

Dates of Interest:

Aug. 23	Classes Begin
Sep. 16	Midterm Exam
Oct. 12	Final Exam, TBD

Grading - Grades will be based on the following materials and weighting factors:

Problem Sets	40%
Midterm 1	30%
<u>Final Exam</u>	<u>30%</u>
Total	100%

Attendance is highly recommended, as you are responsible for any material covered in class. Class notes will be provided to you but additional material may be introduced at the instructor's discretion. You are responsible to knowing about any announcements made in class. We will attempt to simulcast and record all lectures and make them available via the "zoom" tab on the course Carmen site (<http://Carmen.osu.edu>).

Assignments are due to the course instructor by the date and time indicated and will be graded. Problem Sets will be due on the day and time indicated. If you have to miss class, you are still responsible for turning your assignment in on time. You can upload your homework to Carmen. Late assignments will be assessed a penalty. 20% will be deducted from all late assignments, and an additional 10% will be deducted for each day past the due date the assignment is late. If you have extenuating circumstances, the late penalty can be reduced at the discretion of the course instructor. You are encouraged to work with you classmates on homework, but each person must turn in their own assignment.

Exams will be held as listed above. You are responsible informing Dr. Schultz prior to the exam of any conflicts. Reasonable conflicts, as determined by Dr. Schultz, will be accommodated.

Course Reading will be posted as the course progresses. You are expected to read the posted material and be prepared to discuss the topic as we go over it in class. The reading is intended to supplement and emphasize the material we will cover in lecture. When reviewing your class notes, the readings are an excellent resource to clarify questions. It is important to keep up with in class material, as we may get ahead or behind in the schedule.

Policies:

Health and safety requirements: All students, faculty and staff are required to comply with and stay up to date on all university safety and health guidance (<https://safeandhealthy.osu.edu>), which currently includes wearing a face mask in any indoor space. Non-compliance will be warned first, and disciplinary actions will be taken for repeated offenses. These requirements are subject to change.

Disability Services: The University strives to make all learning experiences as accessible as possible. If you anticipate or experience academic barriers based on your disability (including mental health, chronic or temporary medical conditions), please let me know immediately so that we can privately discuss options. To establish reasonable accommodations, I may request that you register with Student Life Disability Services. After registration, make arrangements with me as soon as possible to discuss your accommodations so that they may be implemented in a timely fashion. SLDS contact information: slds@osu.edu; 614-292-3307; slds.osu.edu; 098 Baker Hall, 113 W. 12th Avenue.

Academic Misconduct: Any material submitted (HW, Exams) must represent your own work. Apparent violations of this standard will be referred to the University Committee of Academic Misconduct (COAM) as required by Faculty Rules. It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term “academic misconduct” includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct <http://studentlife.osu.edu/csc/>.

Availability of Mental Health Resources: As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance or reduce a student’s ability to participate in daily activities. The Ohio State University offers services to assist you with addressing these and other concerns you may be experiencing. If you or someone you know are suffering from any of the aforementioned conditions, you can learn more about the broad range of confidential mental health services available on campus via the Office of Student Life’s Counseling and Consultation Service (CCS) by visiting ccs.osu.edu or calling 614-292-5766. CCS is located on the 4th Floor of the Younkin Success Center and 10th Floor of Lincoln Tower. You can reach an on call counselor when CCS is closed at 614-292-5766 and 24 hour emergency help is also available through the 24/7 National Suicide Prevention Hotline at 1-800-273-TALK or at suicidepreventionlifeline.org.

Statement on Sexual Misconduct / Relationship Violence: Title IX makes it clear that violence and harassment based on sex and gender are Civil Rights offenses subject to the same kinds of accountability and the same kinds of support applied to offenses against other protected categories (e.g., race). If you or someone you know has been sexually harassed or assaulted, you may find the appropriate resources at <http://titleix.osu.edu> or by contacting the Ohio State Title IX Coordinator at titleix@osu.edu

Diversity, Equity, and Inclusion: The Ohio State University affirms the importance and value of diversity in the student body. Our programs and curricula reflect our multicultural society and global economy and seek to provide opportunities for students to learn more about persons who are different from them. We are committed to maintaining a community that recognizes and values the inherent worth and dignity of every person; fosters sensitivity, understanding, and mutual respect among each member of our community; and encourages each individual to strive to reach his or her own potential. Discrimination against any individual based upon protected status, which is defined as age, color, disability, gender identity or expression, national origin, race, religion, sex, sexual orientation, or veteran status, is prohibited.

Dr. Schultz's Suggestions for Success:

1. Preview/read the chapters to make yourself familiar with what will be covered in the coming class.
2. Go to class and take notes!
3. Review the notes you take in class – do they make sense?
 - a. If your notes don't make sense, read the relevant chapter in the text
 - b. If the text doesn't help, go to office hours and get help

It is most helpful if you do this sooner rather than right before the exam. If you can't make it to office hours, make an appointment.

4. Do the homework, all of it.
 - a. The homework is supposed to be challenging, it is okay if you struggle
 - b. If you struggle with the homework, review your notes and the relevant portions of the text.
 - c. If you are still stuck, come to office hours or make an appointment. This does require that you do your homework prior to the night before it is due.
5. Prepare for exams.
 - a. Go over your notes and the homework, this is where the test comes from. Try to teach the material to your pillow, if you struggle go back to the notes and the textbook and seek assistance.
 - b. The text provides information in excess of what is covered in class, reading the text is only helpful to understand topics that are unclear in the notes and homework.
 - c. There are additional problems in the text that are unassigned, see if you can work those to test your learning.

Bibliography of helpful resources:

Quantitative Chemical Analysis, by Harris

Data Analysis for Chemistry, by Hibbert and Gooding

Applications of Microsoft Excel in Analytical Chemistry, by Crouch and Holler

Chemometrics: Data Analysis for the Laboratory and Chemical Plant, by Brereton

Chemometrics Tutorial: for PLS_Toolbox and Solo, by Wise, Gallagher, et al.

Analytical Sciences Digital Library, <https://home.asdlib.org/>

MatLab Documentation, <https://www.mathworks.com/help/matlab/>

Additional primary literature and other readings will be provided and links posted on the Carmen course website.

This list is by no means exhaustive, but represents starting points for further learning.